



1st Juli 2013

Simulators:

Kim Lefmann (KU)

Sonja Holm (KU)

Mads Bertelsen (KU)

PSI:

Jürg Schefer

Nadir Aliouane

Mogens Christensen

Center for Materials Crystallography
iNANO & Department of Chemistry

Aarhus Universitet

PAUL SCHERRER INSTITUT



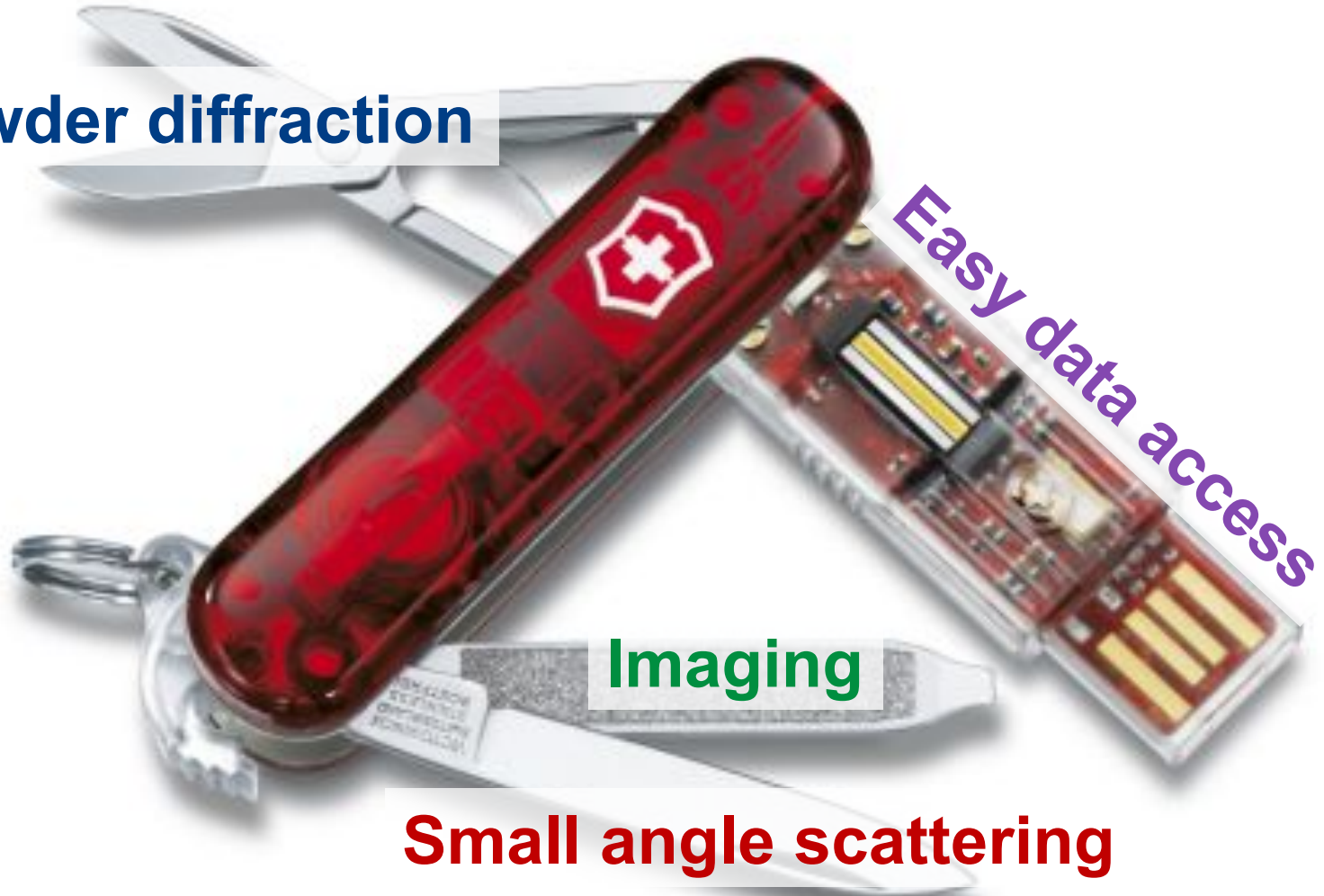
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Avoid over engineering

Combining too many tools makes too many compromises

Powder diffraction

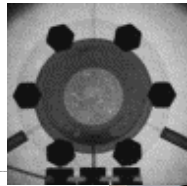
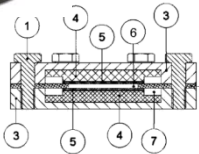


Focus on selected tools and easy data access.

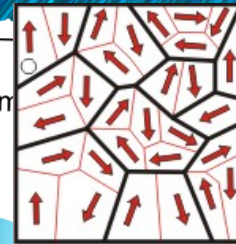
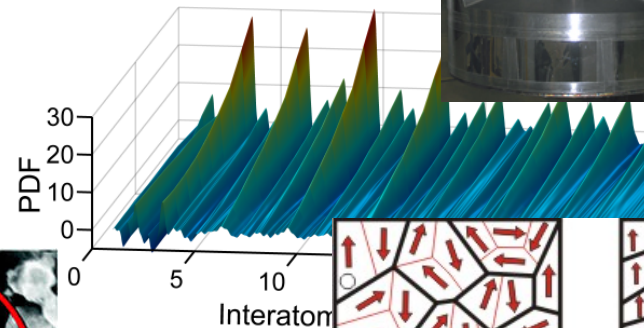
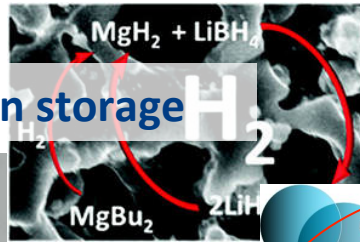
- Light elements and energy related materials.
- Composites, scaffolds or matrix embedded systems.
- Phase transition and nucleation.
- Materials with magnetic properties.



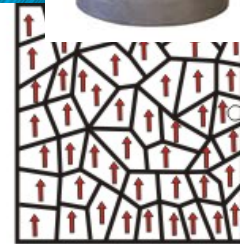
Lithium ion batteries



Hydrogen storage

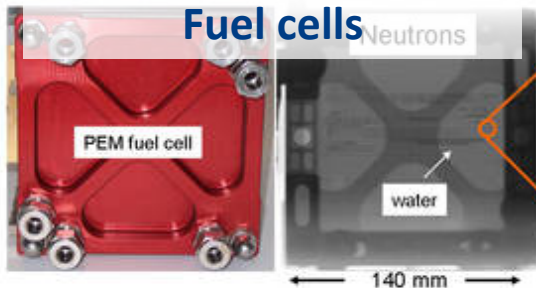


Bulk sample



Compacted nanoparticles

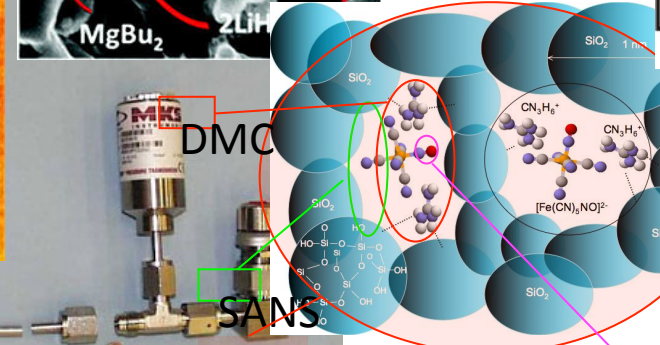
Fuel cells



Neutrons

water

140 mm

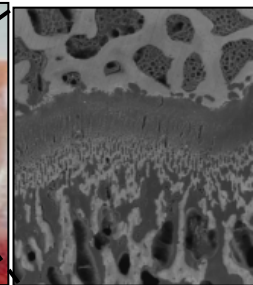
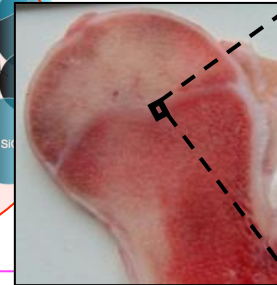


DMC

SANS

ESS Hybrid

MS/HRPT



The idea of combining **SANS** and **NPD** is not unique:

J-Parc has build three instruments:

Nova, I-Materia, HI-SANS

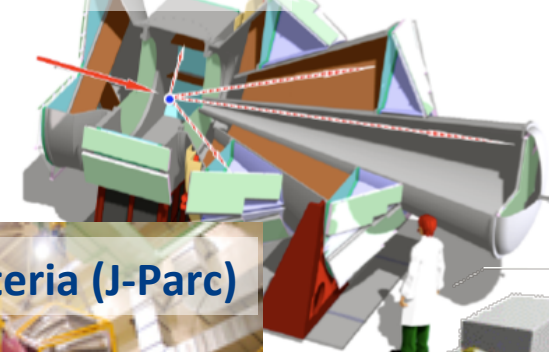
ILL have **D16** – not simultaneous coverage.

SNS planned **SANS** with diffraction detectors.

ISIS have **Nimrod**.

ISIS are building an Instrument for
NI and **NPD** at TS-2: **IMAT**

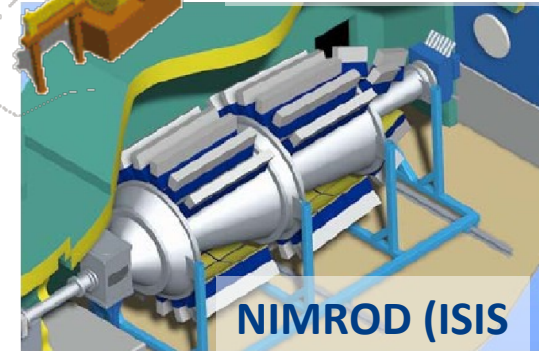
NOVA (J-Parc)



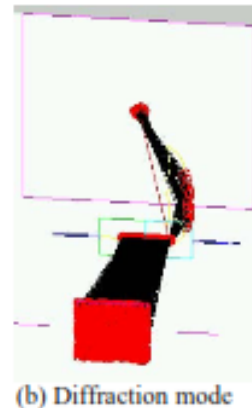
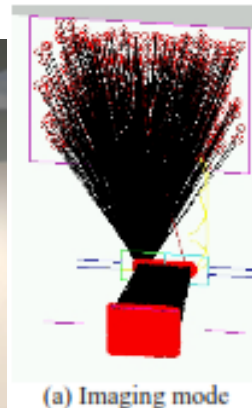
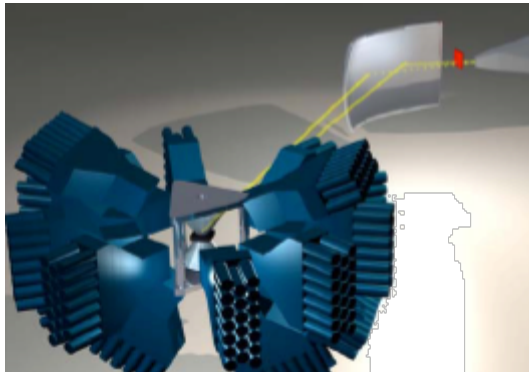
iMateria (J-Parc)



HI-SANS (J-Parc)



NIMROD (ISIS)



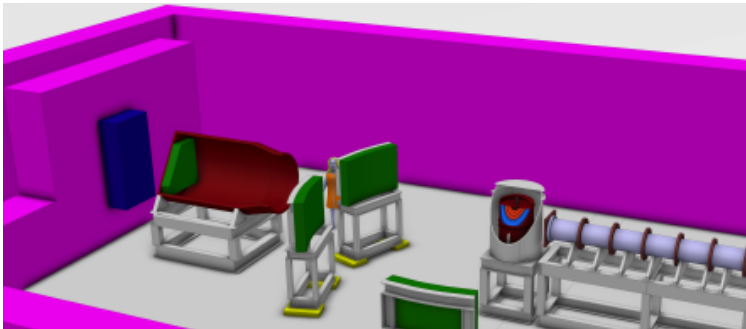
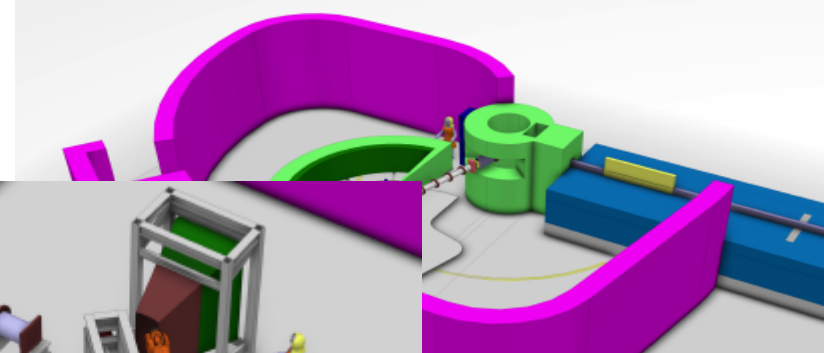
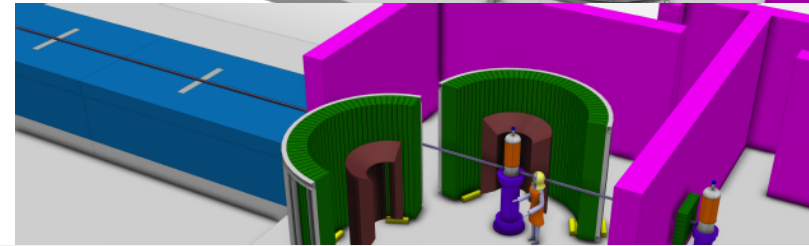
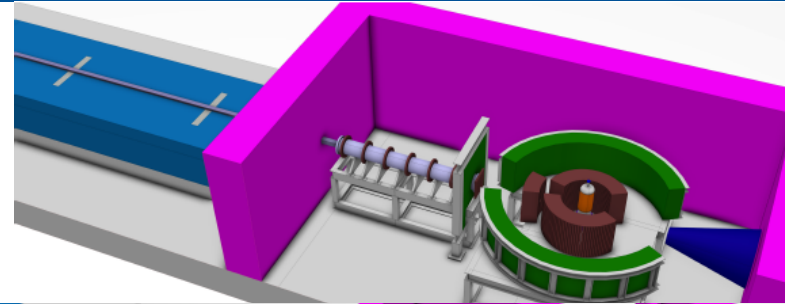
Thermal powder diffractometer

Bispectral powder diffractometer

Pulsed monochromatic powder diffractometer

Materials science & engineering diffractometer

Extreme conditions instrument



TDR v3

HEIMDAL disappeared from the TDR...

Cover multiple length scales:

| Technique | Diffraction | Small angle scattering | Imaging |
|----------------------------|-------------|------------------------|------------|
| Length scale (approximate) | 0.01-5 nm | 1-200 nm | 0.05-50 mm |

Requires large coverage in reciprocal space:

| Technique | Diffraction | Small angle scattering | Imaging |
|--|--------------------------|-----------------------------|---------|
| Reciprocal space (q) | 0.5-20 \AA^{-1} | 0.001-0.2 \AA^{-1} | NA |
| Wavelength band ($\Delta\lambda$) | 0.6-4 \AA | 4-12 \AA | NA |
| Resolution ($\Delta\lambda/\lambda$) | <0.5% | <10% | NA |

Powder diffraction favors:

Short wavelength = high q
 Long instrument = resolution
 Divergent beam = high flux
 Can live with a narrow band

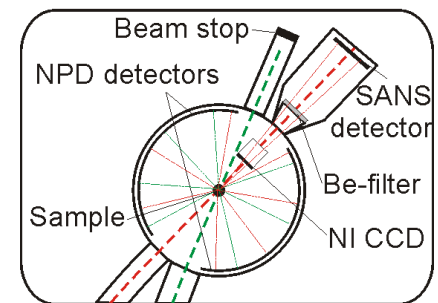
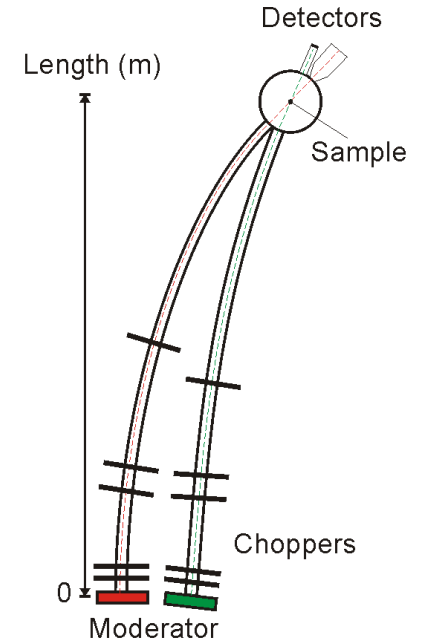
Small angle scattering favors:

Long wavelength = low q
 Short instrument = broad band
 Collimated beam = low q
 Can live with low resolution

Instrument designers and potential users were invited for 2½ day workshop



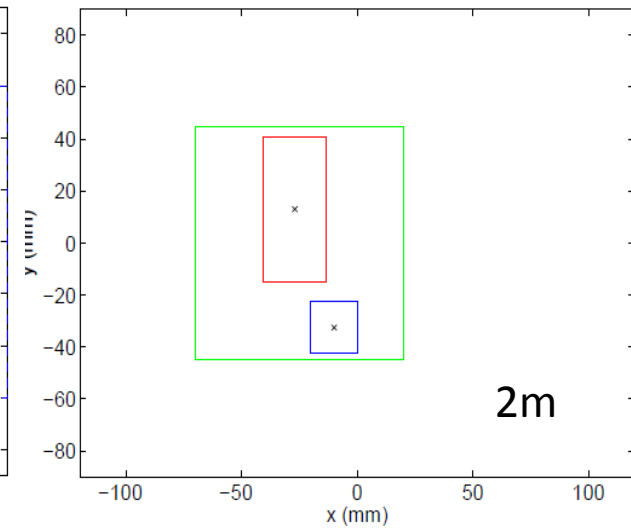
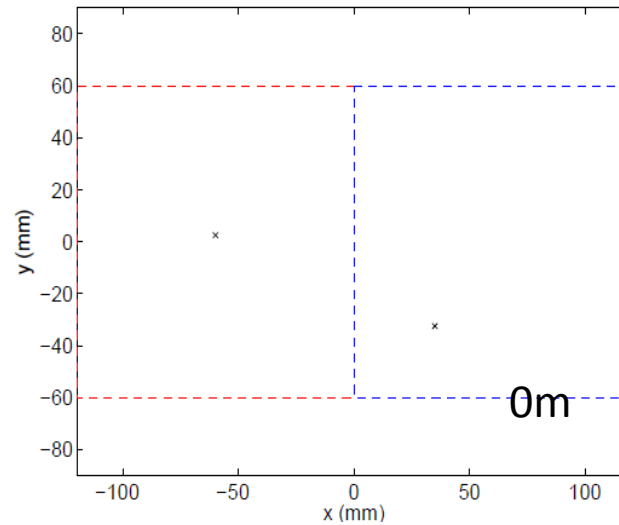
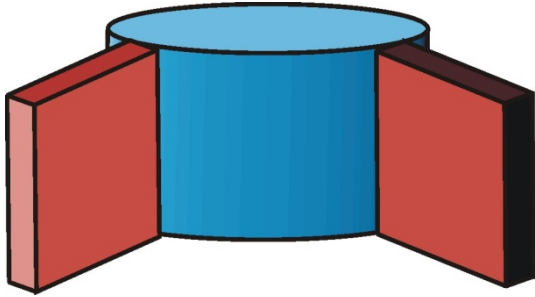
2 guides are needed



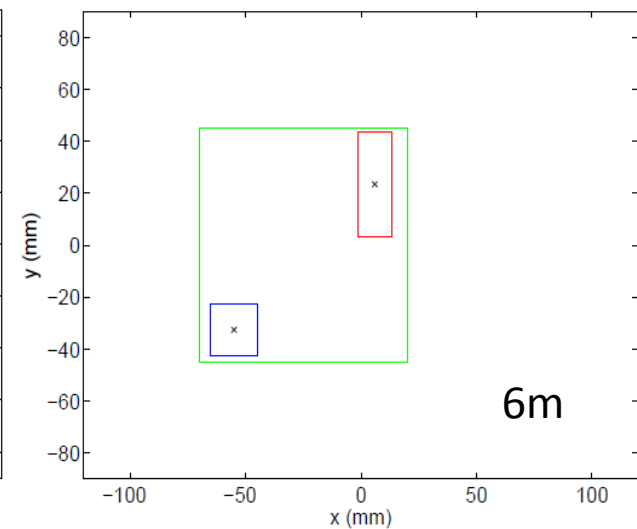
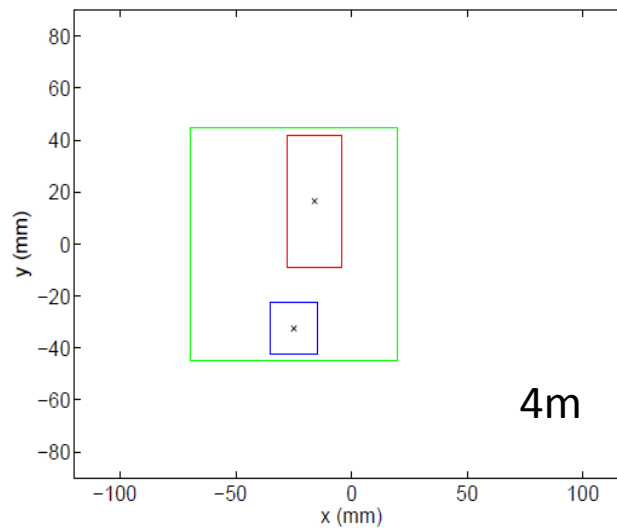
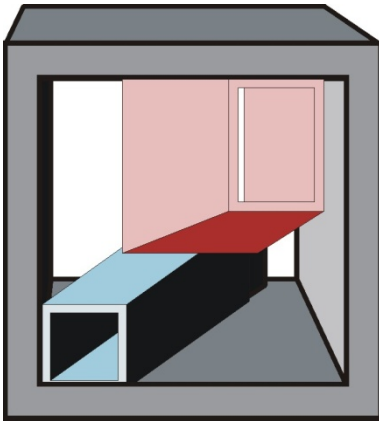
Conclusion from workshop in September 2011

Two guides from a single beamport

Moderator design



Beam extraction



Relative large curvature ($R = 660$ m) on cold guide

The beams meet at an angle of 5°

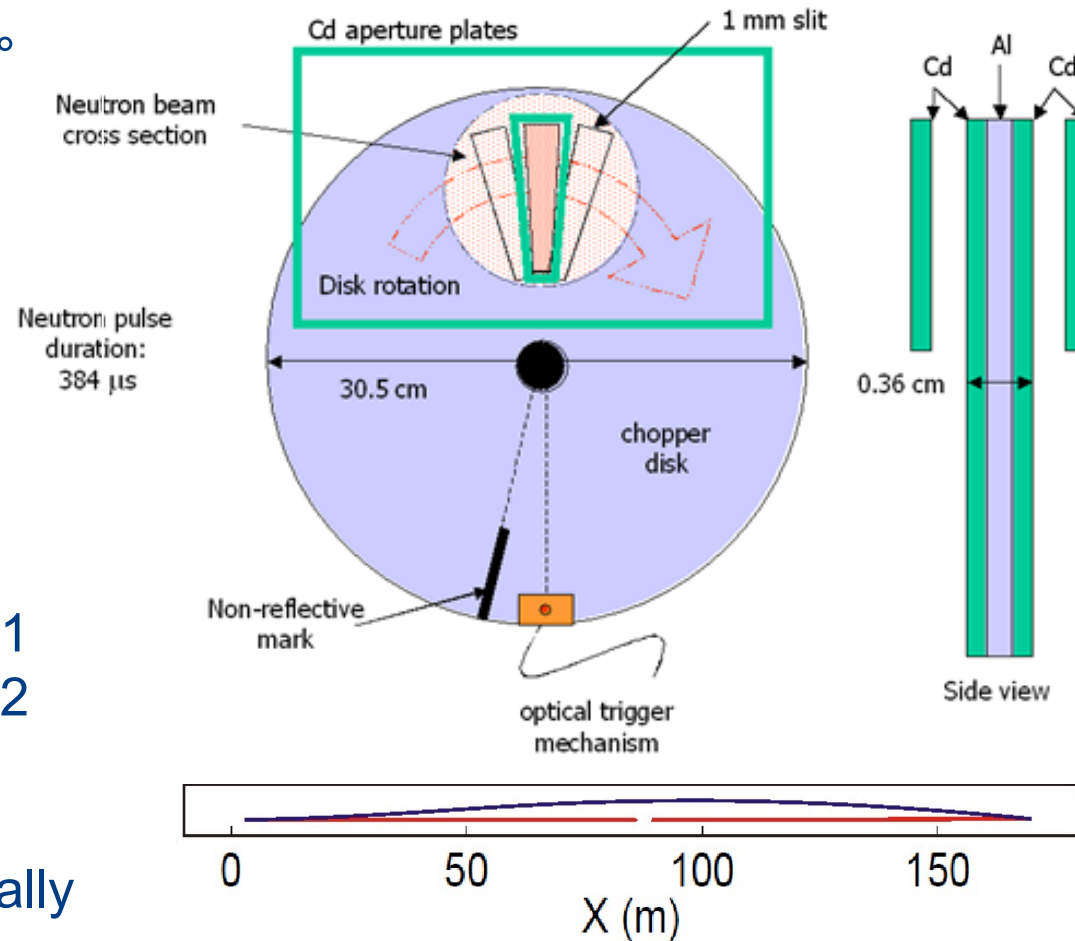
Thermal beam:

- Pulse shaping chopper
- Pulse selection chopper
- Frame overlap chopper

Cold beam:

- Band definition chopper
- Frame overlap chopper #1
- Frame overlap chopper #2

Guides can be optimized individually



Pulse shaping chopper:

- Counter rotating double chopper
- Position: 6.5 from thermal moderator
- Frequency 280 Hz
- $dt_{\min} = 120 \mu\text{s}$ (4%), $dt_{\max} = 724 \mu\text{s}$ (25%)

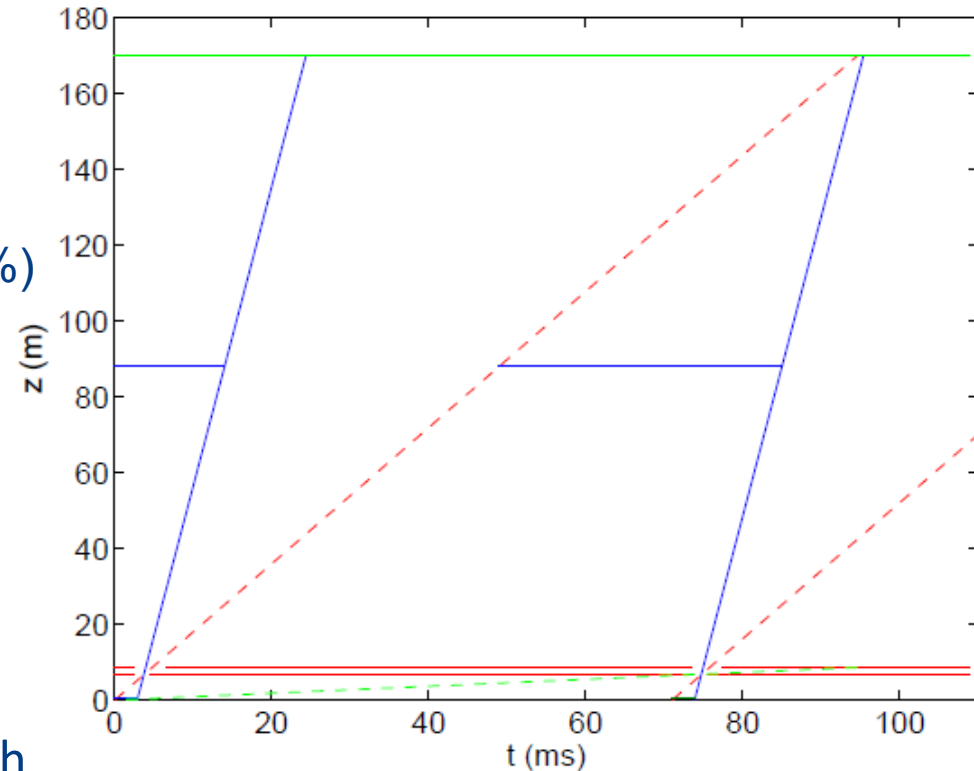
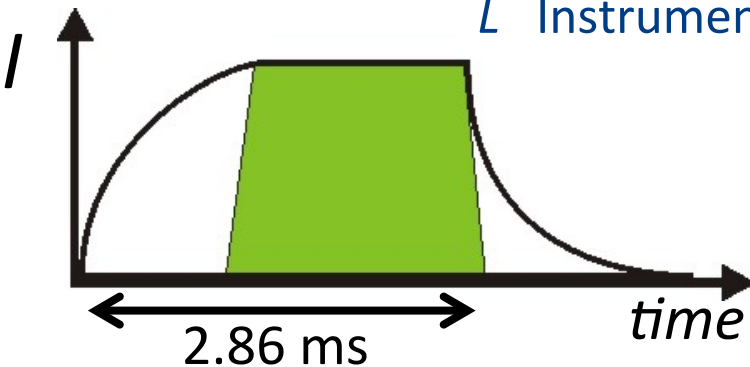
The long pulse allow
trading **flux** for **resolution**

$$\Delta d/d = \tau(\alpha L \lambda)^{-1}$$

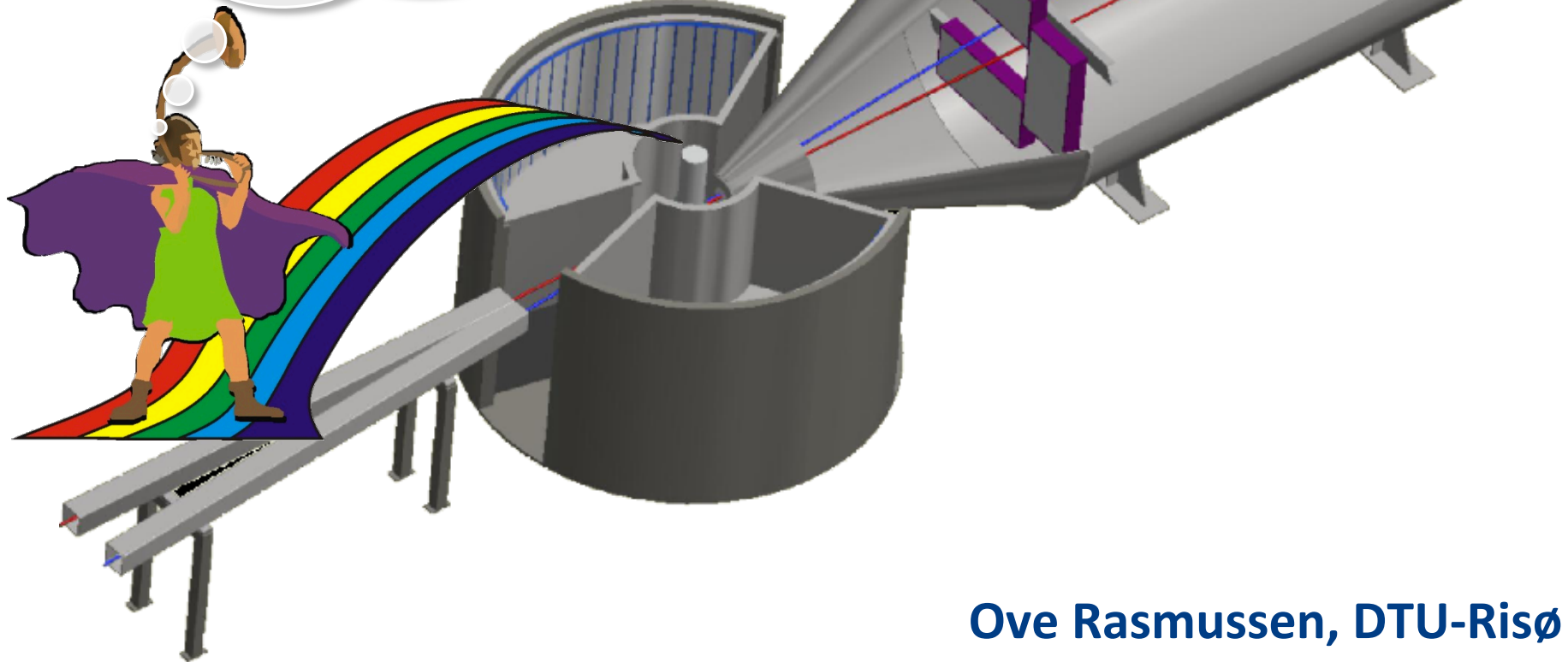
τ pulse length

λ wavelength

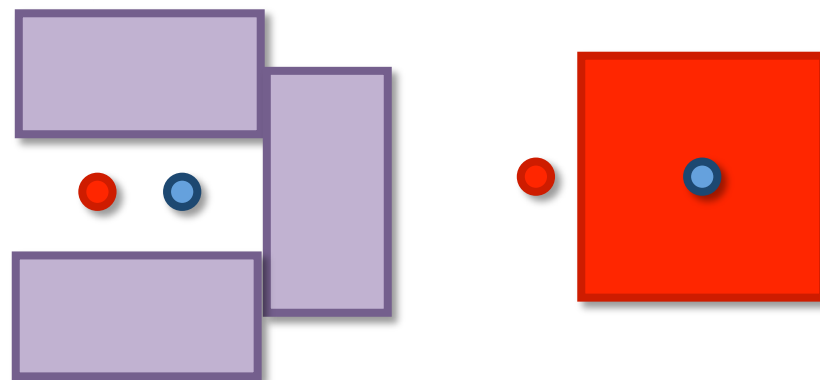
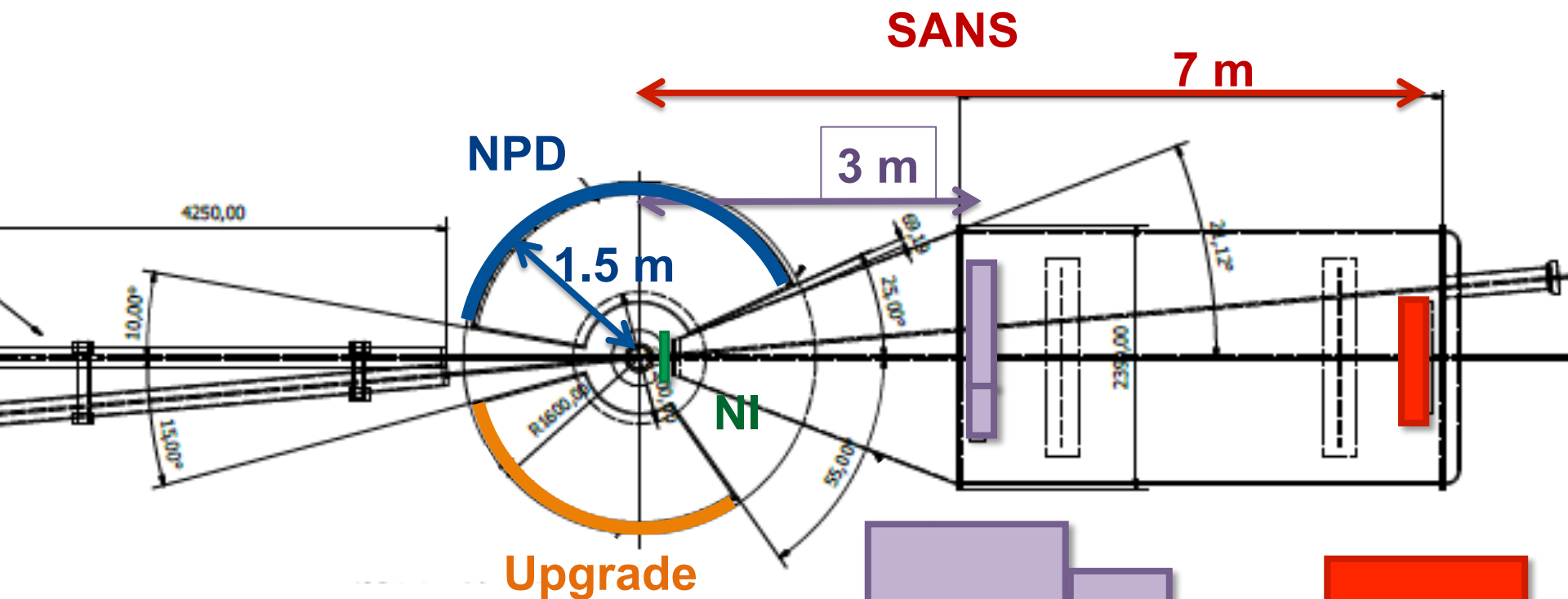
L Instrument length



I see in the dark and
I can hear the grass grow



Ove Rasmussen, DTU-Risø



Q-range coverage:

Cold: 4-5.7 Å: $3 \cdot 10^{-4} - 3 \text{ Å}^{-1}$

11-12.7 Å: $1 \cdot 10^{-4} - 1 \text{ Å}^{-1}$

Thermal: 0.6-2.3 Å: $0.6 - 21 \text{ Å}^{-1}$

Ove Rasmussen, DTU-Risø

Sample access:

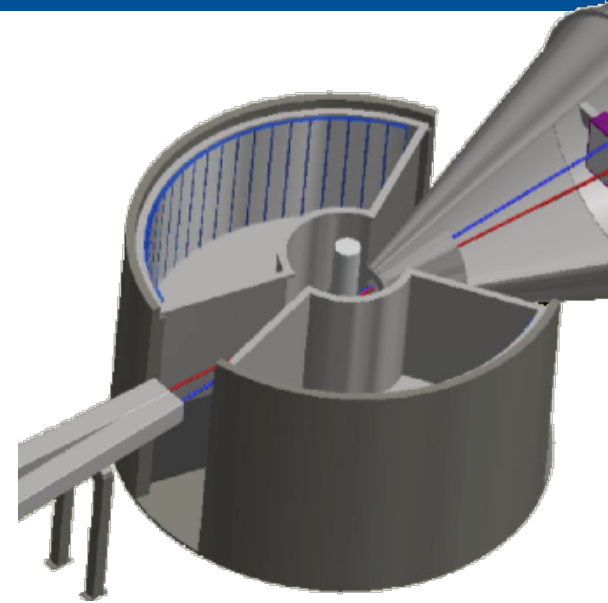
From top and bottom + side

Sample positioning:

X, Y, Z, ω

=> collect PND/SANS at different positions

=> tomography of object



Sample environment test:

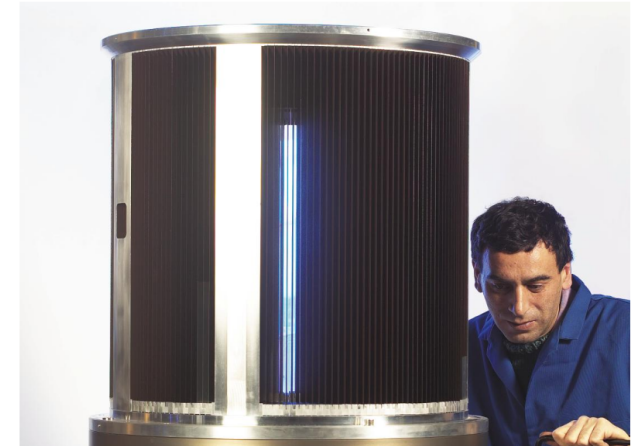
The setup can be build and tested before inserted into instrument.

Integrated optical components:

Radial collimation – different collimation

- Easy insertion/removal

Focusing optics

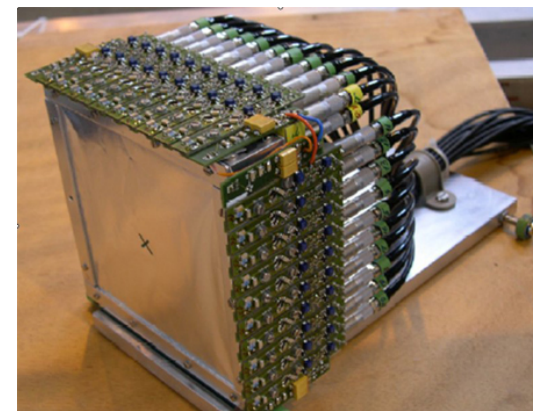


Powder diffraction:

Scintillation detectors with avalanche-photo-diodes

Efficiency – roughly 75% of ^3He detector

Pixel size: $3 \times 10 \text{ mm}^2$ Area $\sim 4 \text{ m}^2$



SANS:

Flat panel detector – based on ESS ^{10}B development

Efficiency – remains to be clarified

Pixel size: $5 \times 5 \text{ mm}^2$ Area $\sim 2.5 \text{ m}^2$



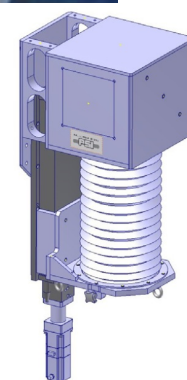
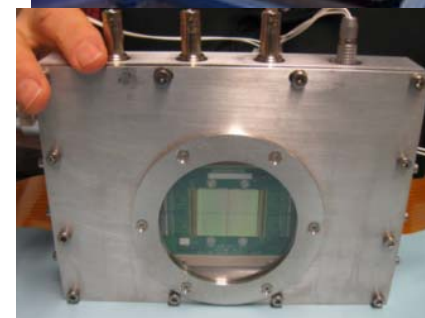
NI:

Medipix – time resolved imaging detector:

Area: $28 \times 28 \text{ mm}^2$, pixel $50 \times 50 \mu\text{m}^2$

Scintillation plate, optical mirror and CCD:

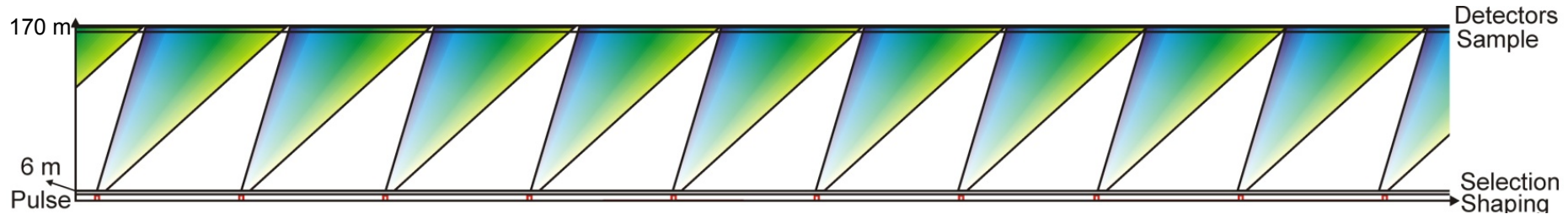
Area: Variable



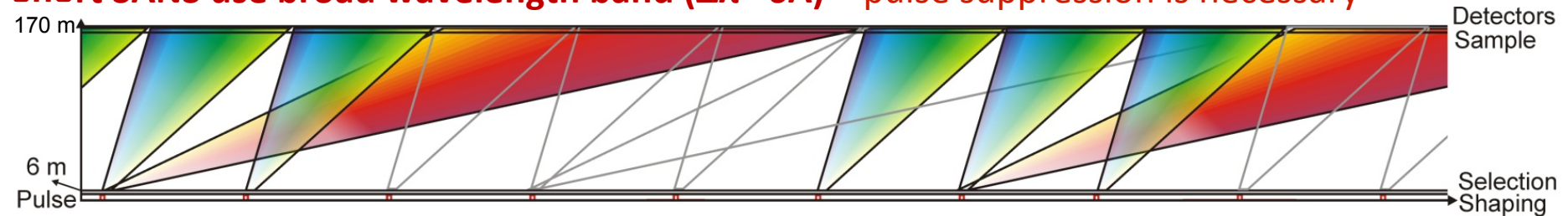
| Investment | Day 1 | Upgrade 1 | Upgrade 2 |
|---|--------------|------------------|------------------|
| Guides (thermal and cold) | 3 | | |
| Shielding HEIMDAL (instrument only) | 1.8 | 0.5 | 0.5 |
| Detectors including support/vacuum chambers | 5.3 | 2.5 | 2.5 |
| Electronics | 0.5 | 0.2 | |
| Sample Area, Instrument Mechanics | 0.6 | | |
| Choppers | 0.5 | | |
| Total HEIMDAL | 11.7 | 3.2 | 2.7 |
| Shielding primary 5° sector | 1.5 | | |
| Total HEIMDAL Sector | 13.2 | 3.2 | 2.7 |
| | | | |
| Personnel | | | |
| Manpower | 1.5 | 0.2 | 0.2 |

SANS related costs: 3.5 M€

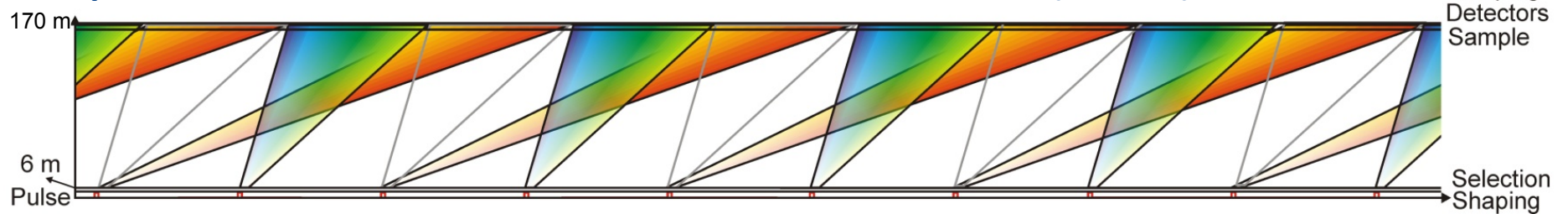
Pure diffraction mode: Thermal powder diffraction (0.6-2.3 Å)



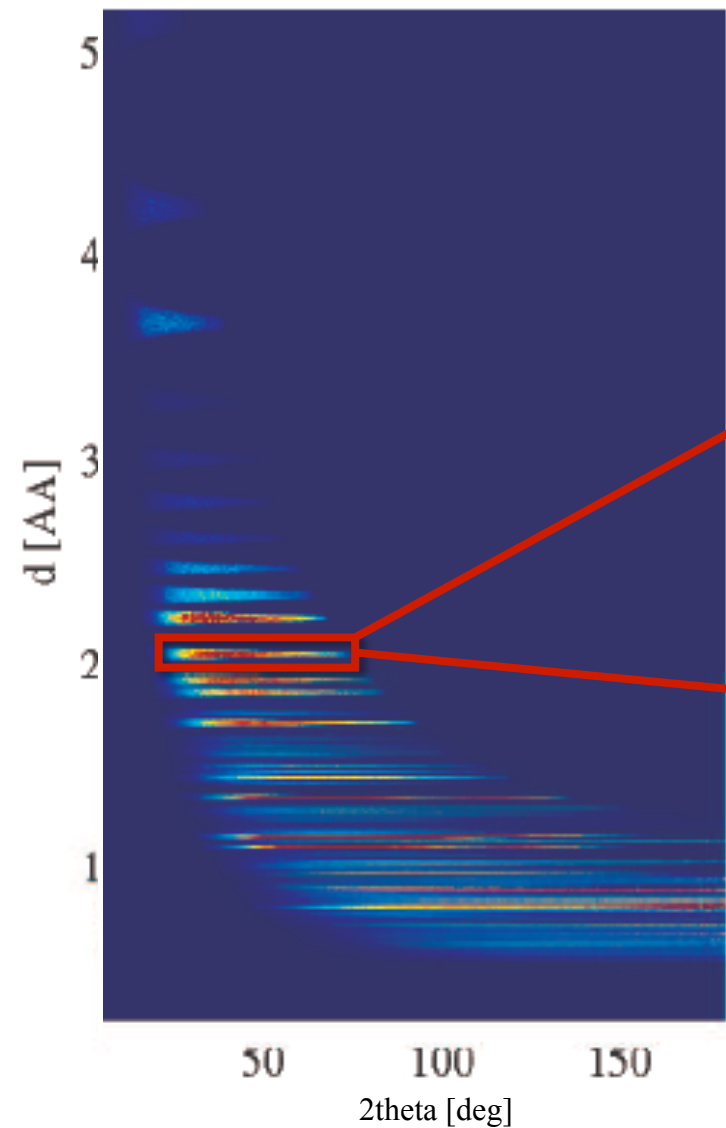
Short SANS use broad wavelength band ($\Delta\lambda \sim 6\text{\AA}$) – pulse suppression is necessary



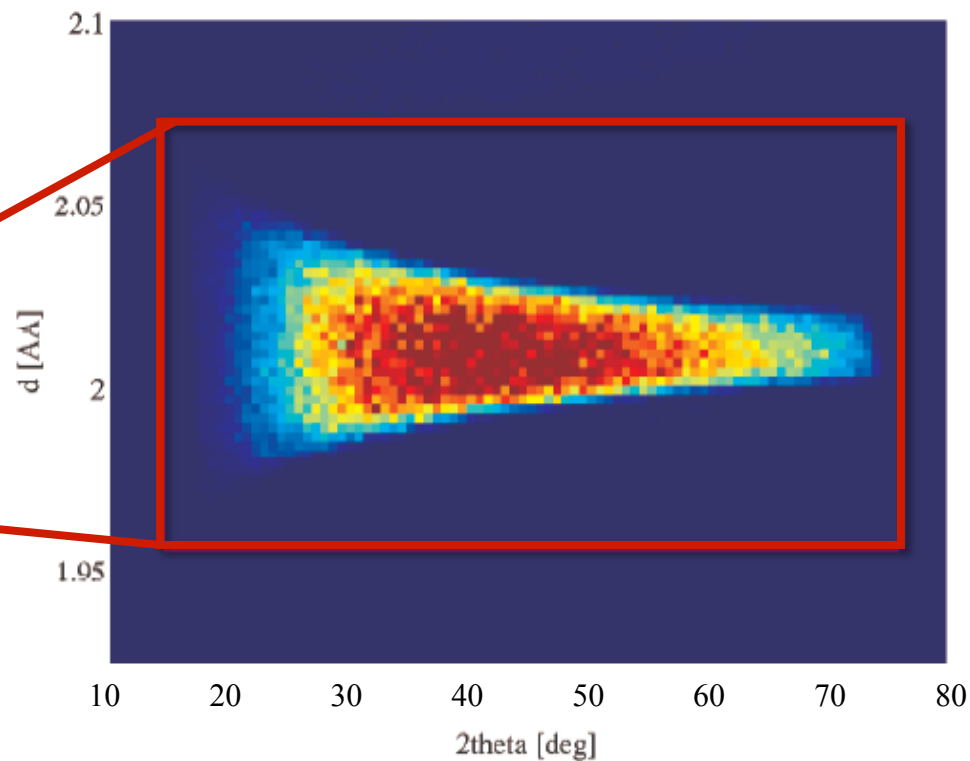
The powder detectors could be used for SANS measurements (4-5.7 Å)



Only single pulse suppression is necessary.



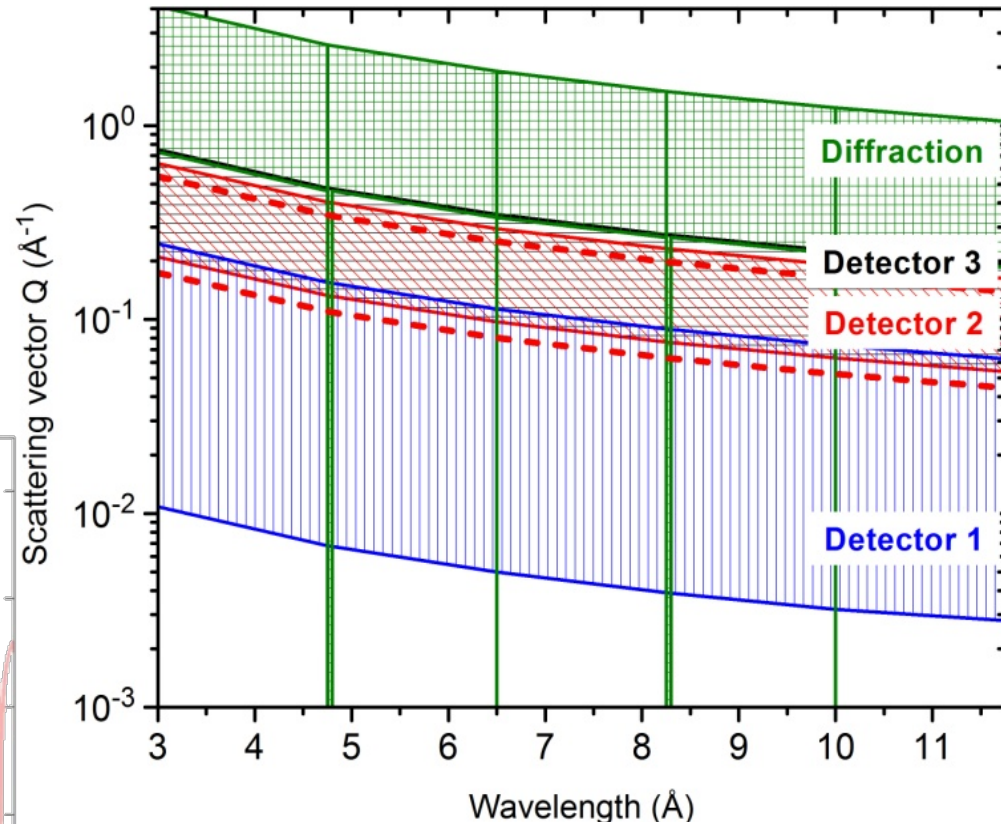
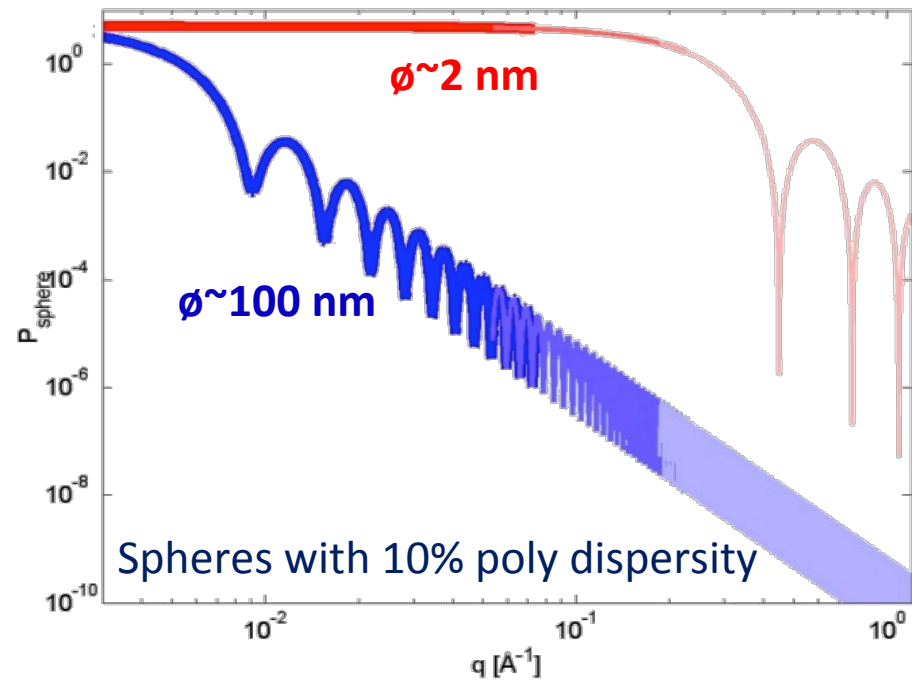
Simulation of Powder diffraction data
2D pattern fitting.



Beamstop:

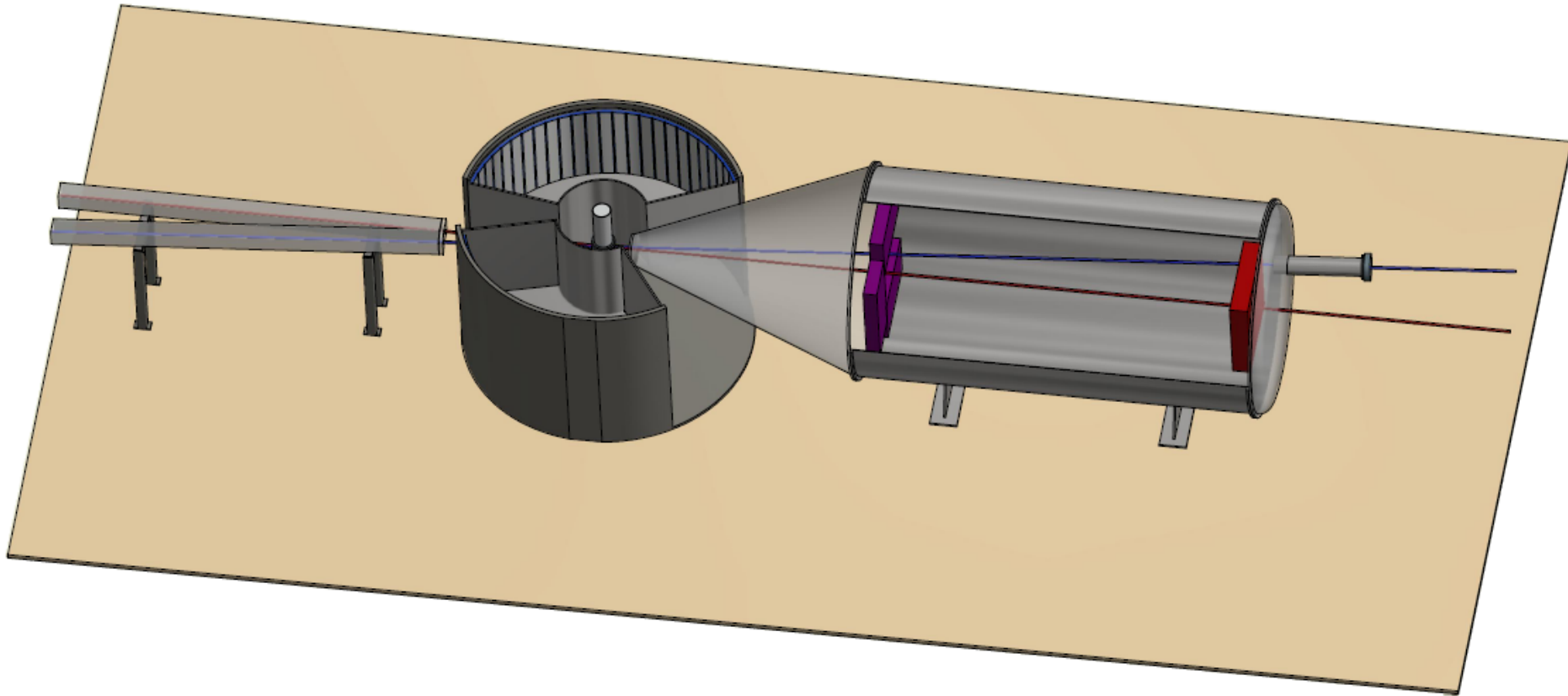
Diameter 3 cm

20 cm from detector



Good Q-range coverage even
with single narrow wavelength band:
 $\Delta\lambda = 10\text{-}11.7 \text{ \AA}$

Should HEIMDAL be a day 1 instrument?



Day 1 instrument? ...Yes

Structure & in-situ processing

Catalytically-active materials

Novel materials

Health & pharmaceuticals

Fuel cells

Battery materials

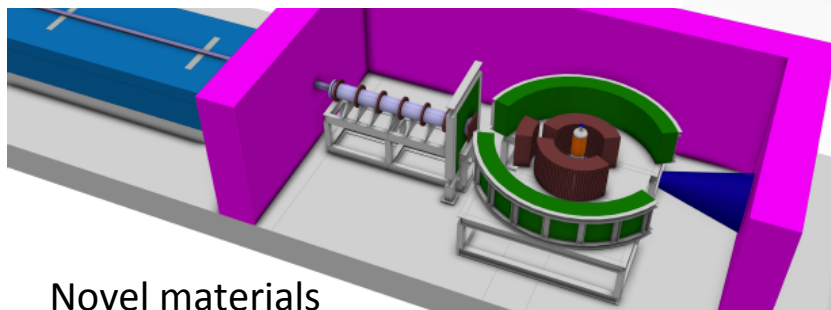
Gas storage materials

Solar cells & photovoltaics

Engineering & geosciences

Archeology & heritage conservation

Thermal powder diffractometer



Novel materials

Structure & in-situ processing

Catalytically-active materials

Fuel cells

Battery materials

Solar cells & photovoltaics

Novel states of matter

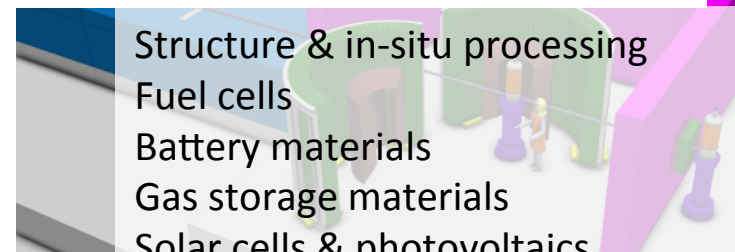
Engineering & geosciences

Archeology & heritage conservation

Earth & environmental sciences

TDR v3

Bispectral powder diffractometer



Structure & in-situ processing

Fuel cells

Battery materials

Gas storage materials

Solar cells & photovoltaics

Catalytically-active materials

Novel materials

Health & pharmaceuticals

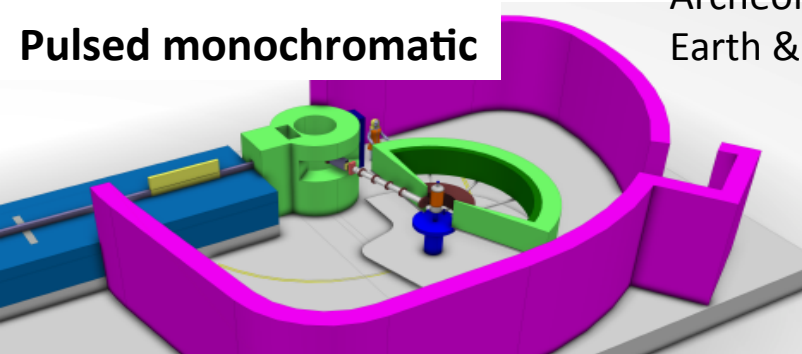
Novel states of matter

Engineering & geosciences

Paleoclimatology & climate change

Earth & environmental sciences

Pulsed monochromatic



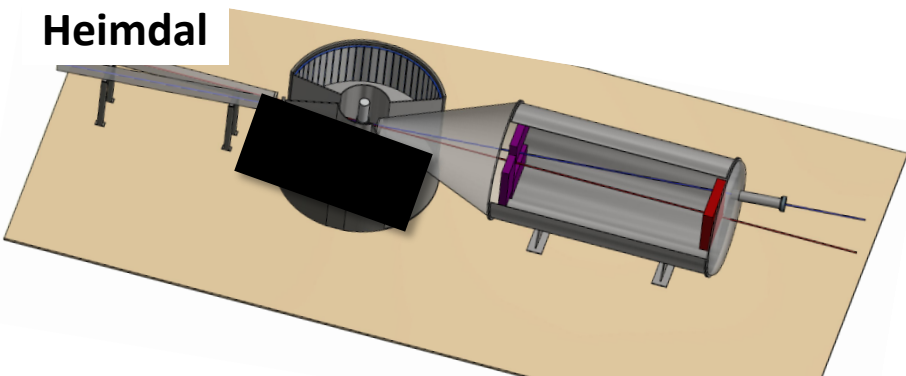
PAUL SCHERRER INSTITUT



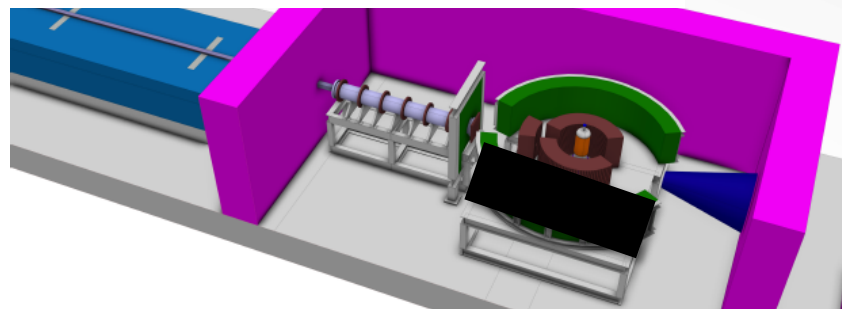
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Heimdal



Thermal powder diffractometer



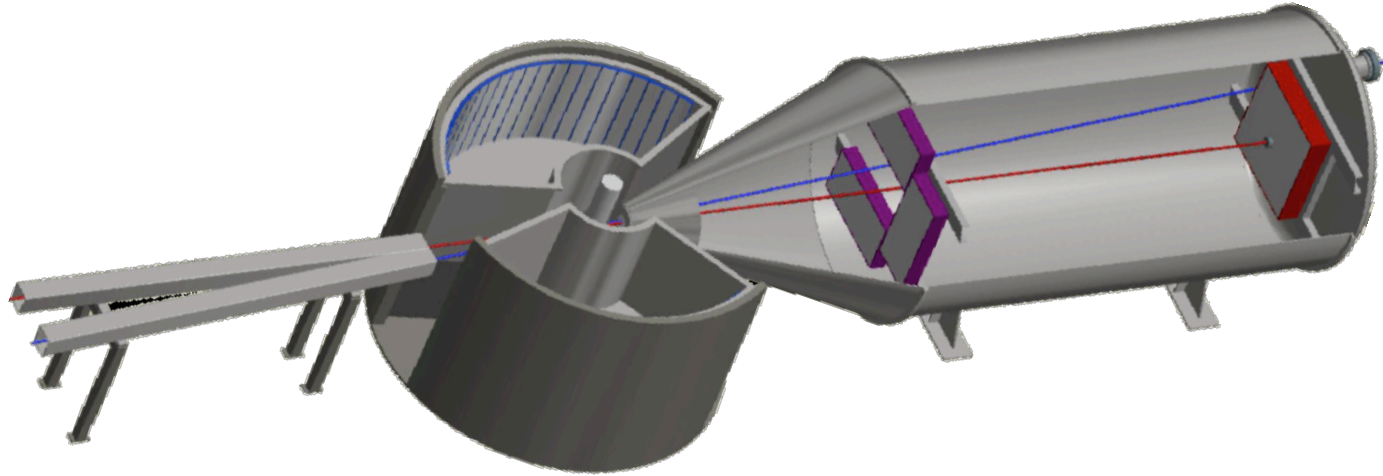
HEIMDAL can cover the same science cases

Plus broader length scales!

A day-1 instrument typically has
1 side covered by detectors
WISH, POWGEN

Structure & in-situ processing
Catalytically-active materials
Novel materials
Health & pharmaceuticals
Fuel cells
Battery materials
Gas storage materials
Solar cells & photovoltaics
Engineering & geosciences
Archeology & heritage conservation

The **pure powder part** of HEIMDAL is identical
to the thermal powder diffractometer.



HEIMDAL is a novel concept:

Allows completely new science

Performance similarly to Thermal Powder Diffractometer

Has the potential to attract new users

How can AU participate in the in-kind process?